

**METABOLOME PROFILING METHODS USING CHROMATOGRAPHIC AND
SPECTROSCOPIC DATA IN PATTERN RECOGNITION ANALYSIS**

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ABSTRACT

Methods are provided that apply neural network technology to recognize small
metabolic changes in microorganisms, plants or animals to detect changes induced by
pesticide (herbicide, insecticide, fungicide) treatment, genetic modification, environmental
10 stress, and other external or internal factors that have influence on metabolite concentrations.
The method implements recognition of nuclear magnetic resonance spectra, mass spectra,
and/or chromatograms of crude plant extracts and association of such spectra or
chromatograms with the treatment of tissue before harvest. The spectra and chromatograms
have information of all the metabolites above a concentration threshold contained in the plant
15 tissue extract. The method applies mathematical models to the very complex plant tissue
extract and allows the detection of treatments with bioregulators such as pesticides, or genetic
modifications such as gene insertions or deletions.

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